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## CHEMICAL REACTING FLOWS

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### ABSTRACT

Future aerospace propulsion concepts involve the combustion of liquid or gaseous fuels in a highly turbulent internal air stream. Accurate predictive computer codes which can simulate the fluid mechanics, chemistry, and turbulence-combustion interaction of these chemical reacting flows will be a new tool that is needed in the design of these future propulsion concepts. Experimental and code development research is being performed at Lewis to better understand chemical reacting flows with the long term goal of establishing these reliable computer codes.

Our approach to understanding chemical reacting flows is to look at separate more simple parts of this complex phenomena as well as to study the full turbulent reacting flow process. As a result we are engaged in research on the fluid mechanics associated with chemical reacting flows. We are also studying the chemistry of fuel-air combustion. Finally, we are investigating the phenomena of turbulence-combustion interaction. This presentation will highlight research, both experimental and analytical, in each of these three major areas.

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## CHEMICAL REACTING FLOWS

Chemical reacting flows of aerospace propulsion systems have features similar to other internal flows described previously. The flows are typically highly turbulent, with large secondary flows and three-dimensional flow characteristics. Flow oscillations and unsteadiness is usually noticed in these flows. There are additional features which are unique to flows with combustion which adds a great deal of complexity to the process. This includes a substantial increase in temperature as the flow moves downstream, and a significant change in fluid properties due to fluid species changes. In addition, the time scale for combustion is often orders of magnitude different than the fluid flow time, and there is often a strong interaction between the turbulent flow and the combustion process. These complex features not only make experimental studies difficult but also significantly affect the methods for computing these flows with computer codes.

## CHEMICAL REACTING FLOWS

### HAS FEATURES OF INTERNAL FLOWS:

- TURBULENT
- HIGHLY THREE-DIMENSIONAL
- FLOW UNSTEADINESS

### HAS ADDITIONAL COMPLEXITY:

- SUBSTANTIAL HEAT RELEASE
- MANY CHANGE OF SPECIES
- COMBUSTION TIME  $\ll$  FLOW TIME SCALE
- FLOW—COMBUSTION INTERACTION

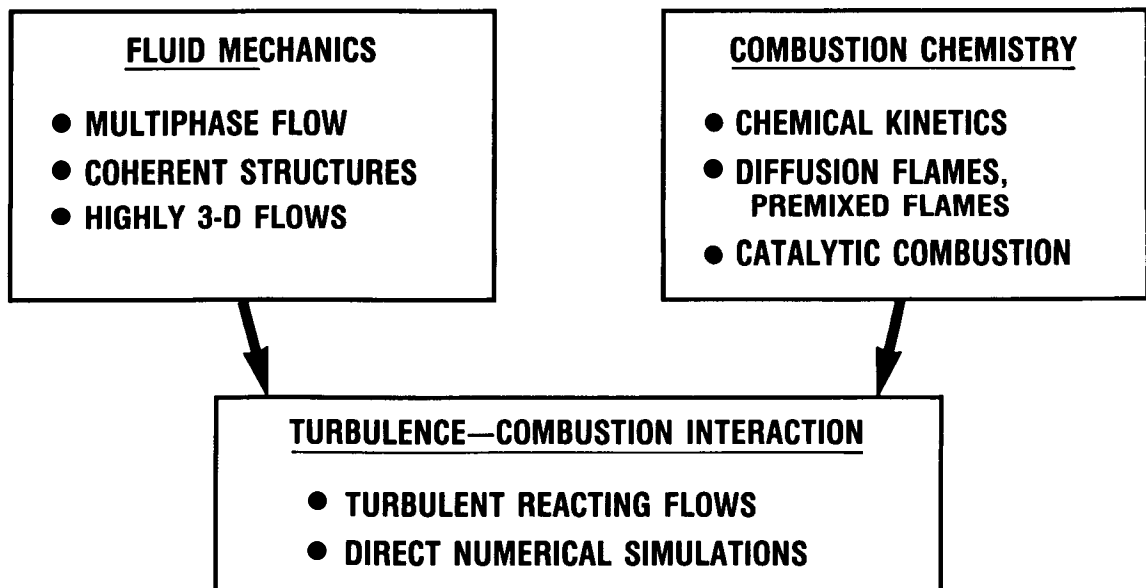
## CHEMICAL REACTING FLOWS

The research activities in chemical reacting flows are divided into three areas as follows: (1) Fluid Mechanics, which looks at the fluid flow phenomena associated with combustion without the added complexity of including heat release. This includes the multiphase processes of fuel sprays, and the highly three-dimensional and time varying flows that typically exist in real propulsion systems. (2) Combustion Chemistry, which concentrates on the combustion of fuel and oxidizer without including the fluid mechanics. Research is being done to understand the ignition process of fuel and oxidizer and to probe the detailed chemistry to obtain an accurate combustion model for further fluid codes. Catalytic combustion is also being studied as a fuel processor for high speed propulsion. (3) Turbulence Combustion Interaction, which looks at both the fluid mechanics and the chemistry of combustion and their effects on each other. Work is being done to understand the key features of turbulent reacting flow and to construct accurate computer codes to simulate this flow. As a useful "numerical experiment," the technique of direct numerical simulation is also being used to better understand chemical reacting flows.

These three major areas of activities are all being performed to achieve the long term goal to obtain an accurate predictive code with coupled fluid mechanics and chemistry which will be helpful in the design of future aerospace propulsion systems.

Let us now look at an example of the research in the area of Fluid Mechanics research on multiphase flow of liquid fuel sprays in air.

## CHEMICAL REACTING FLOWS



**LONG TERM GOAL: ACCURATE PREDICTIVE CODE WITH COUPLED FLUID MECHANICS AND CHEMISTRY FOR FUTURE AEROSPACE PROPULSION**

## MULTIPHASE FLOWS

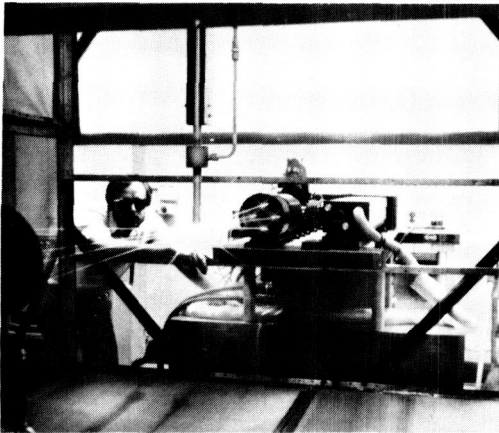
The fuel-spray process is extremely important in terms of engine efficiency, durability, and operability. The ultimate objective of the research is to develop a computer code that can accurately model the fuel and air mixing with subsequent combustion process. Since this is a very complicated process, it is being approached in a series of steps of increasing complexity. Particle-laden jets were initially studied in order to assess the capability of current two-phase flow models. Evaporating liquid sprays and then combusting sprays will also be studied.

## MULTIPHASE FLOWS

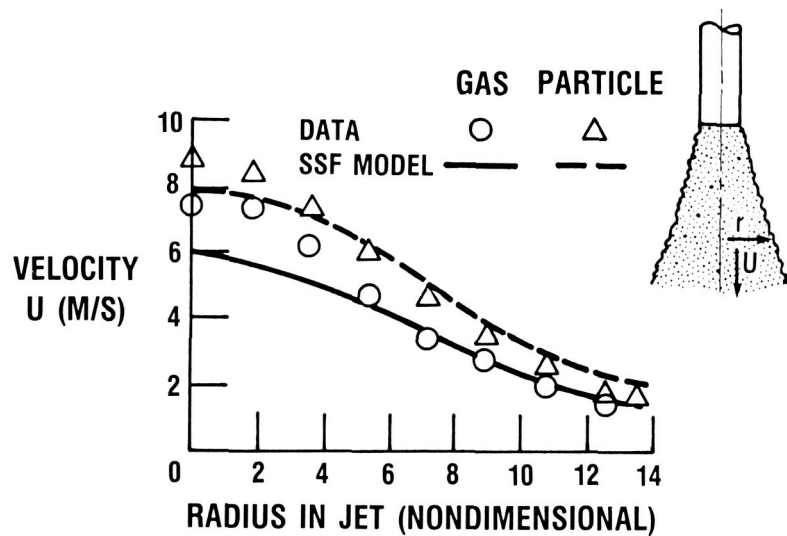
### OBJECTIVE:

DEVELOP COMPUTER CODE WHICH ACCURATELY MODELS FUEL SPRAY/AIR MIXING AND COMBUSTION PROCESSES

### APPROACH:



(1) PARTICLE-LADEN JET EXPERIMENT



(2) TWO-PHASE FLOW COMPUTER MODELS

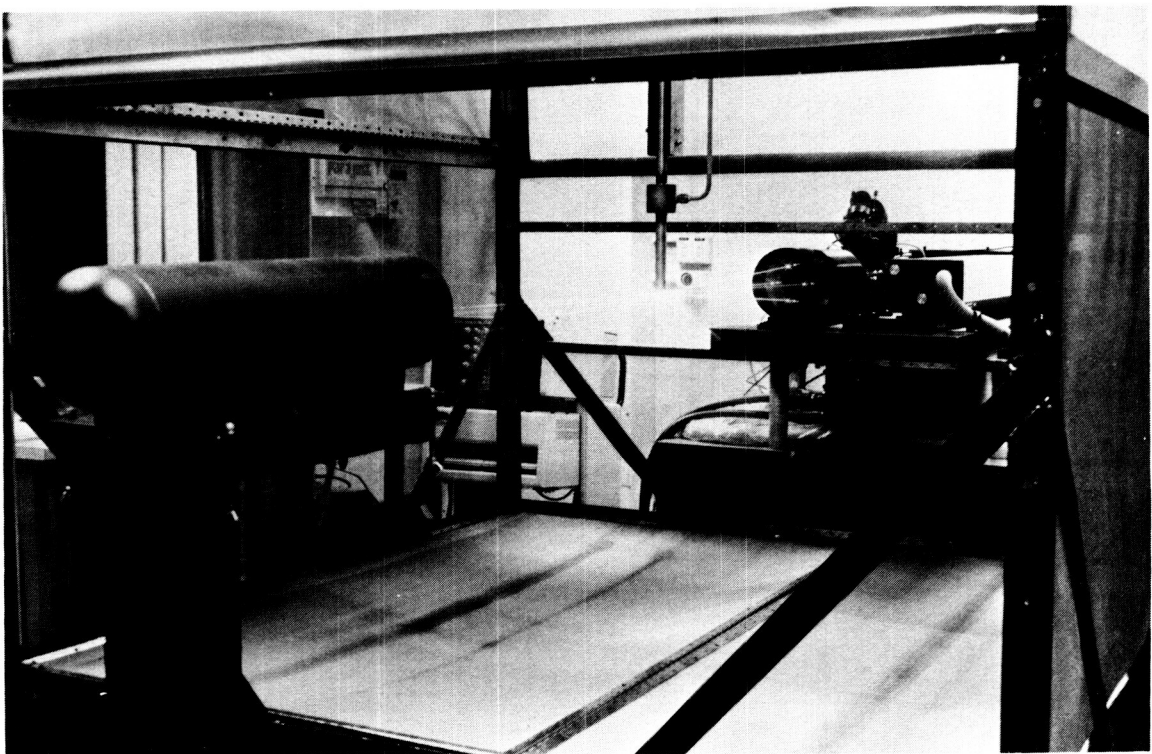
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#### PARTICLE-LADEN SWIRLING FLOW EXPERIMENTAL STUDY

This photograph illustrates the experimental arrangement of the particle-laden jet. An air jet containing solid glass beads (39 micron, Sauter Mean Diameter) discharged downward into a still environment. Particle-laden jets with three swirl numbers were studied. Nonintrusive measurements of velocity were obtained with a two-channel laser velocimeter. Particle size and velocity were measured with a phase/doppler particle anemometer. The gas phase was seeded with nominal 1-micron diameter aluminum oxide power to measure gas phase velocities.

#### PARTICLE-LADEN SWIRLING FLOW EXPERIMENTAL STUDY



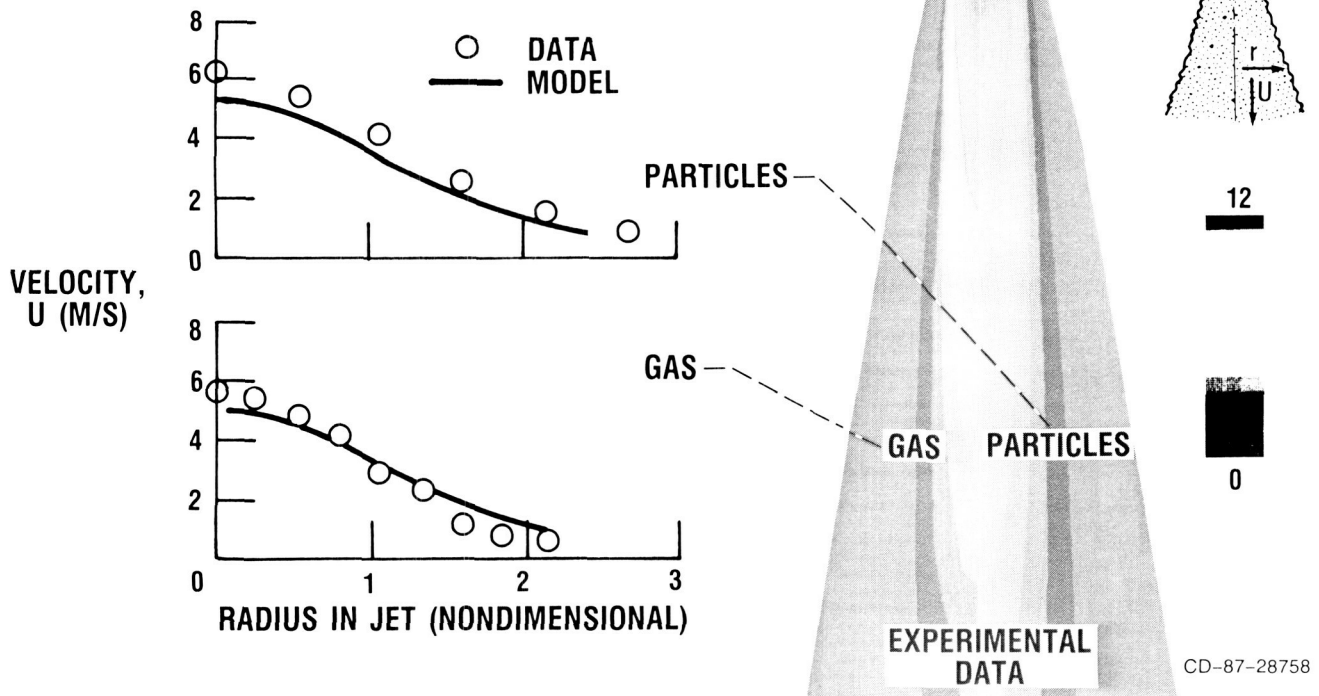
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## MULTIPHASE FLOW VELOCITY COMPARISON

This figure presents typical results from the particle-laden jet study. A contour plot of experimentally measured axial velocity of the gas phase (left side) and particle phase (right side) is illustrated. It is evident that initially, the gas phase has a higher velocity than the particle phase. The particles are initially accelerated by the gas phase and then their velocity begins to decay. Because of their inertia, the rate of decay of axial velocity is slower for the particles than the gas. Also shown in the figure are predictions from the SSF model at 10 diameters downstream of the tube exit. This model tracks particle trajectories in the computed gas phase flowfield and allows momentum exchange between phases. The model also considers effects of gas-phase turbulence on particle trajectories. Predictions from the model show reasonable agreement with the data.

## MULTIPHASE FLOW VELOCITY COMPARISON

- PARTICLE DIAMETER, 39 MICRON (SMD)



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## MULTIPHASE FLOWS

Future directions for multiphase flow research include evaporating liquid sprays and combusting liquid sprays. Evaporating sprays are currently being studied under contract at the University of California, Irvine, and Allison Gas Turbine as part of the HOST Program. The test cell where the particle-laden jets were studied is currently being modified to study liquid sprays.

## MULTIPHASE FLOWS

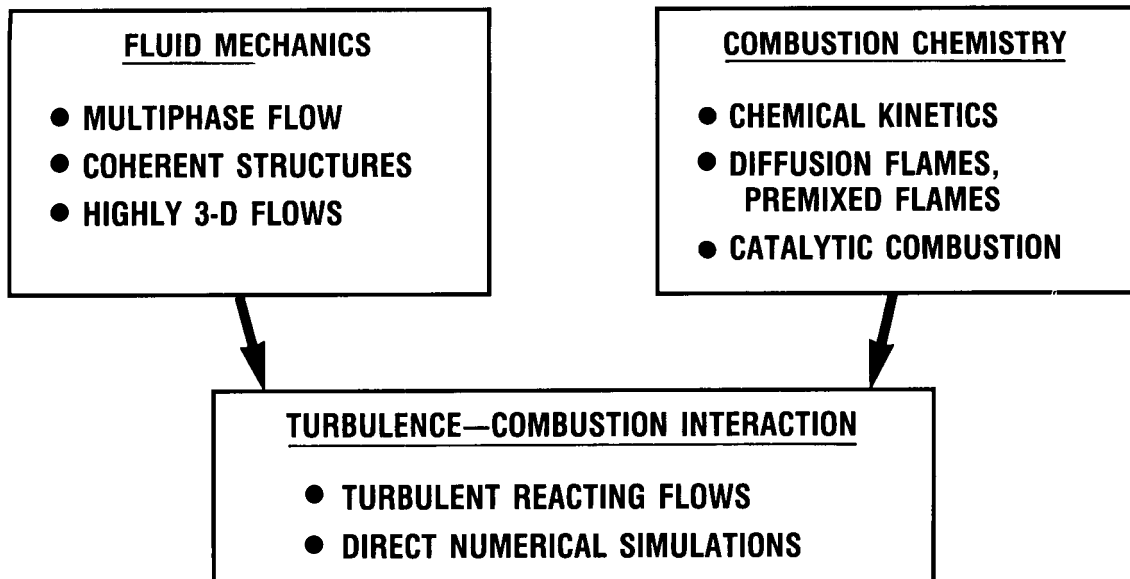
### FUTURE DIRECTIONS:

- (1) EVAPORATING LIQUID SPRAY
- (2) LIQUID FUEL SPRAY COMBUSTION

## CHEMICAL REACTING FLOWS

Let us now turn our attention to the area of Combustion Chemistry. An example of the research in this area is the study of the chemical kinetics of hydrogen-air combustion.

## CHEMICAL REACTING FLOWS



**LONG TERM GOAL: ACCURATE PREDICTIVE CODE WITH COUPLED FLUID MECHANICS AND CHEMISTRY FOR FUTURE AEROSPACE PROPULSION**

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## CHEMICAL KINETICS

In a supersonic ramjet propulsion system, the time required between the injection of fuel into the airstream and its combustion point is very important with regards to the length of the engine and its weight. These high speed combustion concepts will be tested in wind tunnels where the air has been heated to simulate the aerodynamic heating of the vehicle in the atmosphere. Research is underway to determine the combustion delay time of hydrogen fuel and air and to determine the effects of air contaminants in the wind tunnel on this combustion delay time.

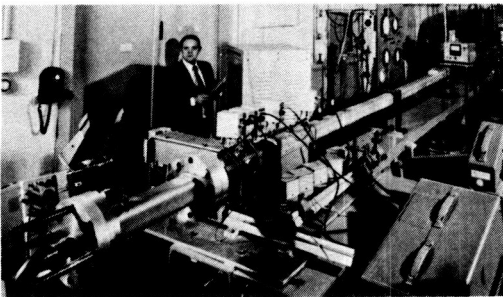
Stoichiometric  $H_2-O_2$  ignition delay times were measured behind reflected shock waves at 1.1 atm pressure over the temperature range 1300 to 950 K by using a chemical shock tube. The proposed chemical kinetic model predicted ignition delay times in excellent agreement with the experimental data.

## CHEMICAL KINETICS

### OBJECTIVE:

DETERMINE COMBUSTION DELAY TIME OF  
HYDROGEN FUEL—AIR CHEMISTRY

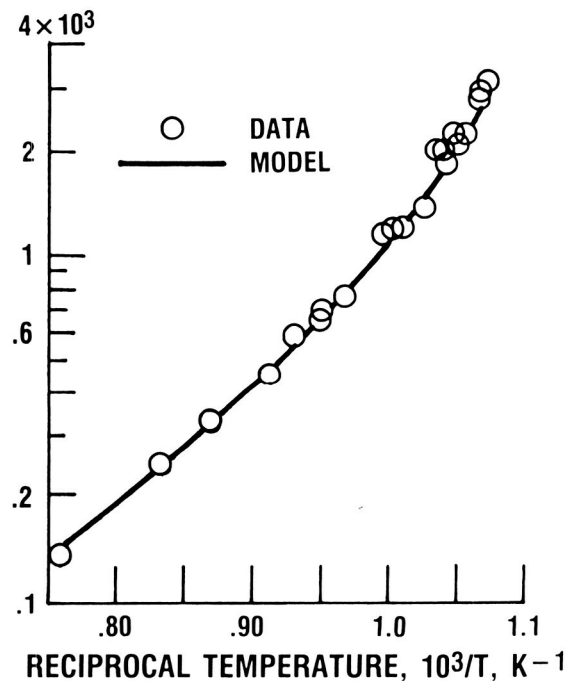
### APPROACH:



(1) CHEMICAL SHOCK TUBE

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COMBUSTION  
DELAY  
TIME,  $\mu\text{sec}$



(2) REACTION RATES COMPUTER MODEL

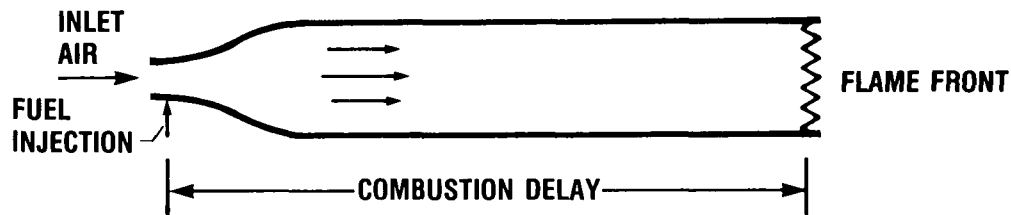
## CHEMICAL KINETICS

The information which we are seeking is to determine how far from the fuel injection point will a stable flame exist in a supersonic airstream of various Mach numbers.

Also, since heated wind tunnels have small amounts of contaminants or additives in the air, we are studying the effects of these contaminants on this combustion delay time.

## CHEMICAL KINETICS

### SCRAMJET ENGINE SCHEMATIC:



- HOW FAR WILL STABLE FLAME BE FROM FUEL INJECTION POINT?
- WHAT IS EFFECT OF AIR CONTAMINANTS OR ADDITIVES ON THIS COMBUSTION DELAY?

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## CHEMICAL KINETICS

Shown here are the levels of four major air contaminants which exist in the two U.S. hypersonic wind tunnels when they are simulating a Mach 7 flight speed. Carbon dioxide and water vapor are known to lengthen the combustion delay time. Nitric oxide and nitrous oxide although orders of magnitude smaller in concentrations, would tend to shorten the combustion delay time.

## CHEMICAL KINETICS

### HEATED WIND TUNNEL AIR CONTAMINANTS

CARBON DIOXIDE .....	6 TO 10 PERCENT
WATER VAPOR .....	13 TO 17 PERCENT
NITRIC OXIDE .....	0.9 PERCENT
NITROUS OXIDE .....	0.025 PERCENT

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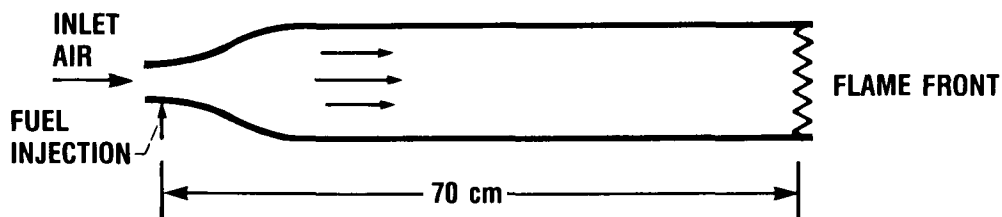
## CHEMICAL KINETICS

Applying the chemical kinetics computer model to the prediction of combustion delay time for a scramjet flying at a Mach 7 flight condition predicted a 70 cm distance between the fuel injection point and the flame front. When the wind tunnel contaminants were taken into account, this distance was significantly shorter: only 13 cm between the fuel injection point and the flame front. Thus, the small concentration of contaminants (nitric oxide and nitrous oxide) resulted in over a factor of five reduction in combustion length. Not only is this effect important in evaluating wind tunnel experiments of combustion concepts, but it also indicates that trace additives into the flow could significantly shorten the required engine length and thereby considerably reduce weight.

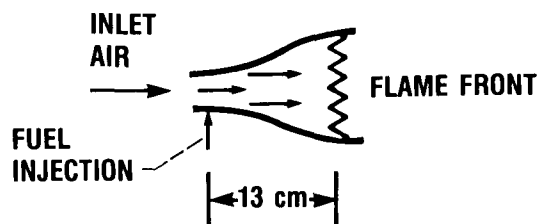
This work is continuing to further explore the effects of these trace contaminants or additives and to better quantify their potential benefit to future scramjet designs.

## CHEMICAL KINETICS

### CALCULATED COMBUSTION DELAY FOR MACH 7 SCRAMJET FLIGHT CONDITION:



(A) BASED ON PURE DRY AIR.



(B) BASED ON PURE AIR WITH CONTAMINANTS OR ADDITIVES.

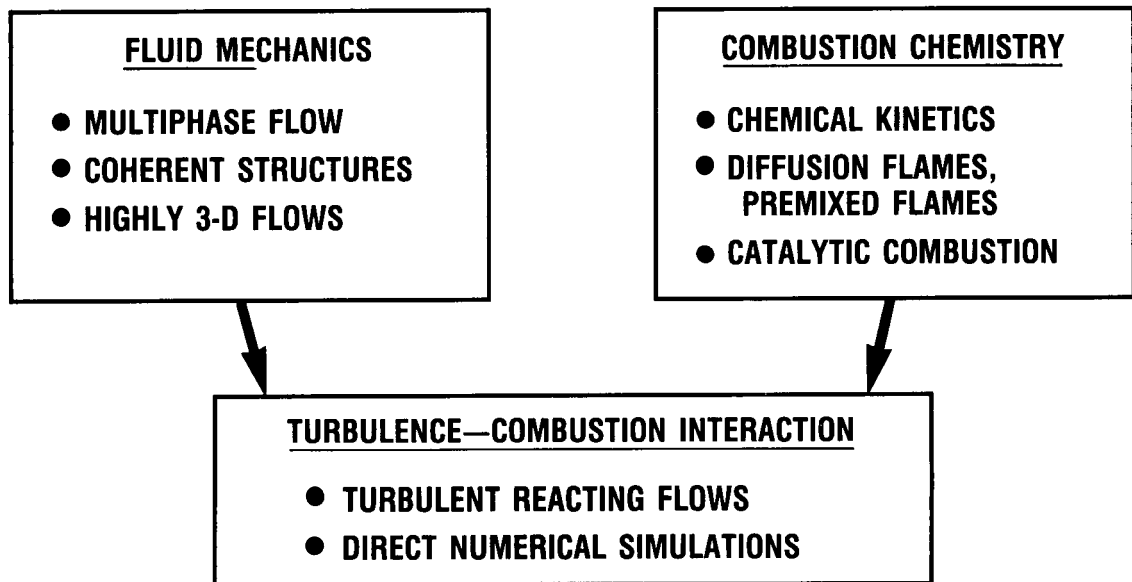
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## CHEMICAL REACTING FLOWS

While it is important and quite useful to look at the fluid mechanics and the combustion chemistry aspects of chemical reacting flows independently, to get a full understanding of the dominant phenomena of these flows, we must examine the interaction of turbulent flow with combustion. The activities in this area include both numerical code development work and experimental research. We will now highlight the research in turbulent reacting flow.

## CHEMICAL REACTING FLOWS



**LONG TERM GOAL: ACCURATE PREDICTIVE CODE WITH COUPLED FLUID MECHANICS  
AND CHEMISTRY FOR FUTURE AEROSPACE PROPULSION**

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## TURBULENT REACTING FLOW

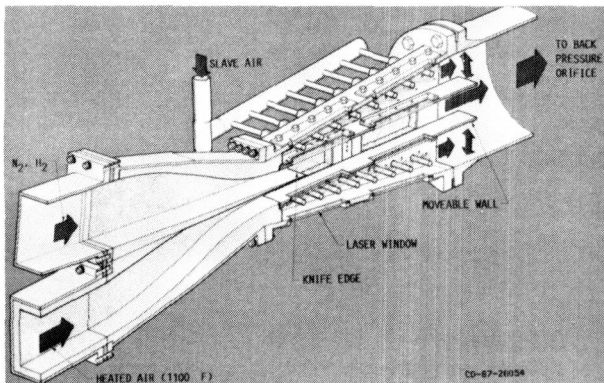
The objective of this work is to understand the coupling between fluid dynamics and combustion and to establish an accurate computer code which simulates the dominant features of turbulent reacting flow. An experiment is being constructed to focus on many of these features, both steady state and unsteady. This experiment is to examine a plane reacting free shear layer. Turbulent reacting flow computer codes, both steady state and time accurate, are also being developed concurrently, and the database from the experiment will serve as a means to validate these new computer codes.

## TURBULENT REACTING FLOW

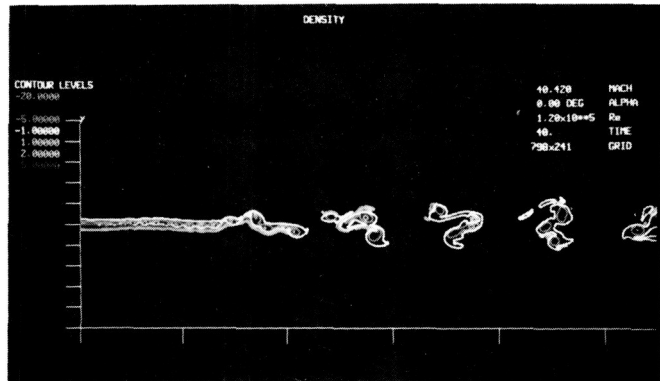
### OBJECTIVE:

**UNDERSTAND COUPLING BETWEEN FLUID DYNAMICS AND COMBUSTION, AND  
ESTABLISH ACCURATE COMPUTER SIMULATIONS OF HIGH-SPEED CHEMICAL REACTING  
FLOW**

### APPROACH:



**(1) REACTING SHEAR LAYER  
EXPERIMENTS**



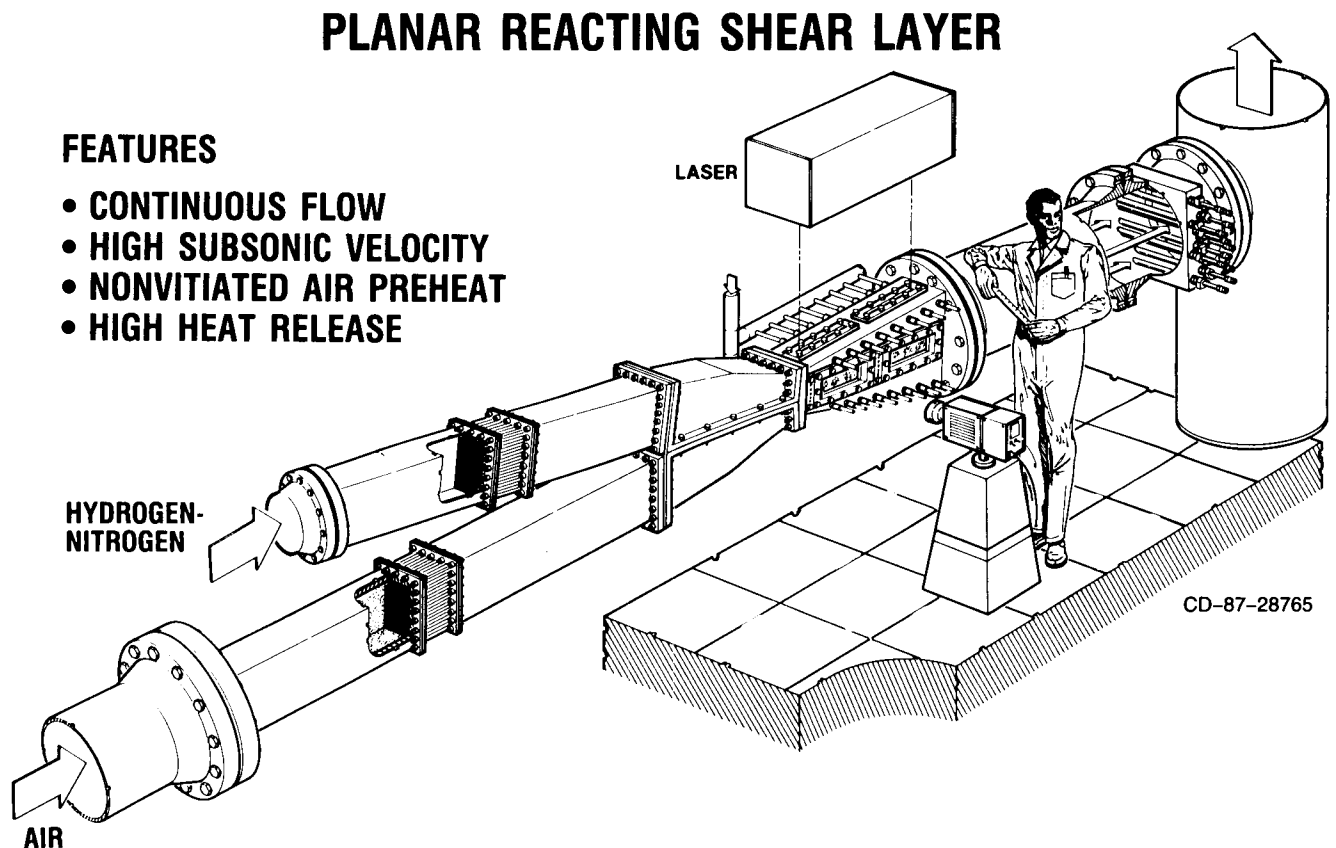
**(2) TURBULENT REACTING FLOW  
COMPUTER CODES**

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## PLANAR REACTING SHEAR LAYER

The objectives of the Planar Reacting Shear Layer Experiment, shown as a schematic here, is to (1) understand the coupling between fluid dynamics and combustion and (2) to establish a data set to validate computer codes which simulate the physics and chemistry of high speed chemical reacting flow. Two gas streams, one of hydrogen and nitrogen, the other of air, will mix downstream of a plane splitter plate. Combustion will occur where the fuel and air has properly mixed. Pressure oscillations in this closed duct will exist due to the dynamic features of the flow and the interactions between these pressure oscillations and the combustng shear layer will be examined. The unique features of this experiment are (1) a continuous flow capability, (2) flow velocities of both the air and the hydrogen-nitrogen mixture which are in the high subsonic range, (3) the air will be heated ahead of the mixing shear layer without any contamination effects, and (4) the heat release in this experiment will be quite high, typical of propulsion systems. The experiment is in fabrication and nonintrusive instrumentation is being purchased. Experiments are expected to begin in spring 1988.



## TURBULENT REACTING FLOW

PROMETHEUS II is a time-accurate version of a two-dimensional, finite volume TEACH code. Second-order accurate QUICK differencing is used for the convective terms and block-correction combined with Stone's strongly implicit algorithm is used to solve the pressure correction equation. This results in a highly efficient computational tool for performing "numerical experiments."

## TURBULENT REACTING FLOW

### TIME-ACCURATE, 2-D SHEAR LAYER CODE

- TWO-DIMENSIONAL NAVIER-STOKES EQUATIONS SOLVED WITH OR WITHOUT A TWO-EQUATION TURBULENCE MODEL
- SECOND-ORDER ACCURACY IN BOTH TIME AND SPACE
- FULLY IMPLICIT NUMERICAL SCHEME DERIVED FROM "SIMPLE" (SEMI-IMPLICIT PRESSURE LINKED EQUATIONS) ALGORITHM

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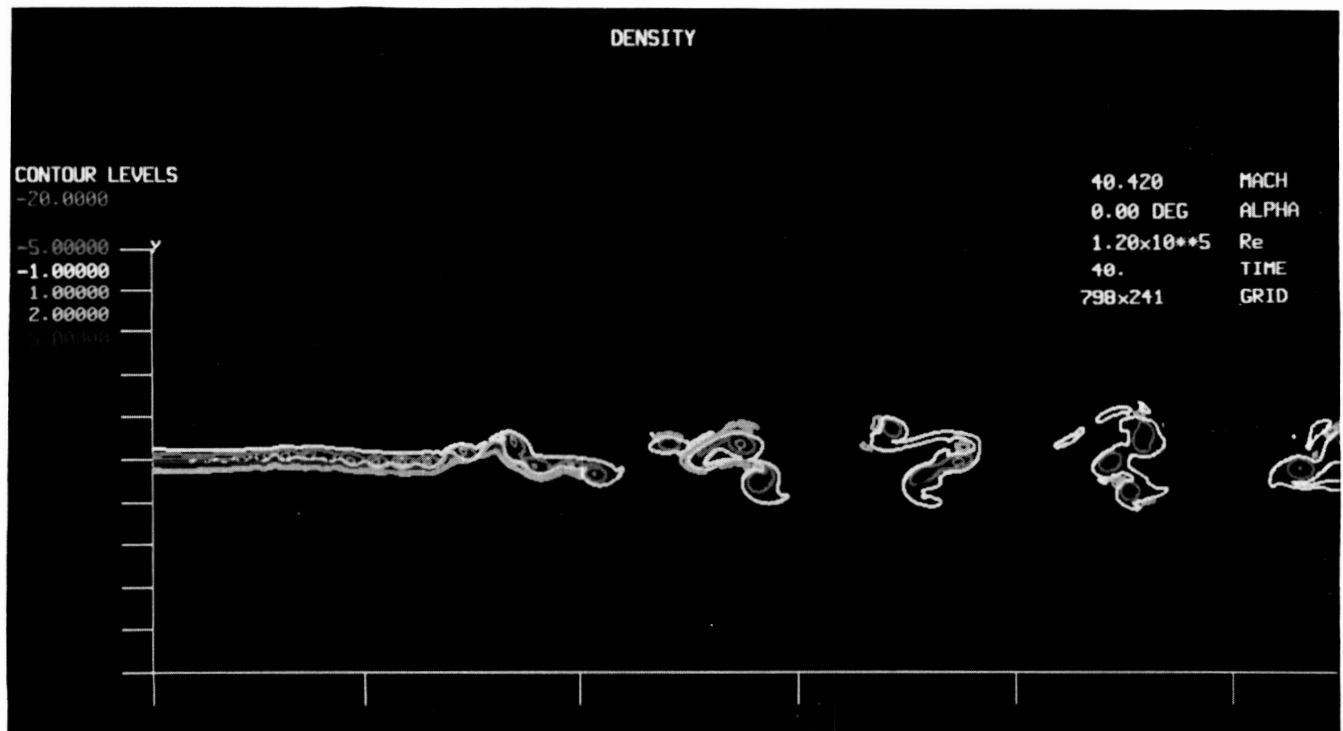
## TURBULENT REACTING FLOW

Shown are vorticity contours for a two-dimensional, numerical calculation of a forced, shear layer at a Reynolds number of about 100,000. The positive and negative vorticity contours originate at the boundary layers, specified at the inlet of the computational domain. Forcing is applied at a long wavelength and smaller scale vorticities spontaneously develop as a result of the natural instability of the layer. These small scale vorticities cluster on the scale of the longer, forced wavelength. Small pockets of positive vorticity persist as remnants of the low speed boundary layer. The collective interaction of these small scale vortices, merging into larger scale structures, largely controls the dynamics of the shear layer. These calculations were performed on the NAS Cray 2 computer.

## TURBULENT REACTING FLOW

### TIME-ACCURATE, 2-D SHEAR LAYER CODE

### COMPUTER CODE RESULTS OF TWO STREAM FREE SHEAR LAYER SHOWING VORTICITY STRUCTURE



## TURBULENT REACTING FLOW

The RPLUS2D code is being developed for calculation of mixing and chemical reactions in the flow fields of ramjets and scramjets. The code is written in generalized curvilinear coordinates and therefore can handle any arbitrary two-dimensional geometry. The implicit LU (lower-upper) scheme used in the RPLUS2D code requires only scalar diagonal inversions while most other implicit schemes require block matrix inversions. The use of scalar diagonal inversions offers order-of-magnitude efficiency improvement over conventional implicit schemes when large systems of partial differential equations must be solved, such as flows in ramjet and scramjet engines. A three-dimensional version of this code will be developed subsequent to the completion of this two-dimensional code.

## TURBULENT REACTING FLOW

### STEADY STATE FLUID MECHANICS COMPUTER CODE:

#### IMPLICIT L U SYMMETRIC GAUSS-SEIDEL ALGORITHM WITH FINITE VOLUME DISCRETIZATION

- MAJOR ADVANTAGE OF ELIMINATING BLOCK INVERSIONS WHERE THE NUMBER OF BLOCKS COULD BE QUITE LARGE FOR REACTING FLOWS
- REAL GAS PROPERTIES
- KINETIC REACTION RATE SOURCE TERMS TREATED IMPLICITLY

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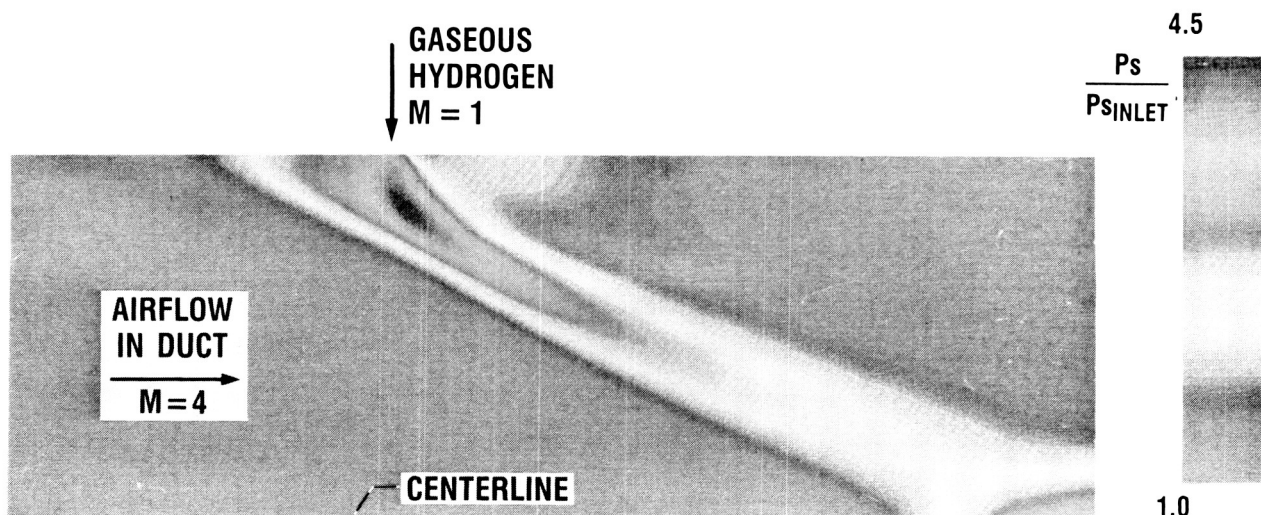
## TURBULENT REACTING FLOW

The  $H_2$  jet injected at right angles to the main airflow acts essentially as an effective body which blocks the flow resulting in a bow shock and strong pressure gradients on the front side of the jet. The jet shock around the injector can also be seen in this figure. The two bow shocks resulting from the two  $H_2$  jets at top and bottom walls (symmetric about the centerline shown) intersect at the center plane and yield a large pressure rise.

## TURBULENT REACTING FLOW

### STEADY STATE FLUID MECHANICS COMPUTER CODE:

COMPUTER CODE RESULTS OF GASEOUS FUEL JET—AIR MIXING AND COMBUSTION IN  
INTERNAL DUCT FLOW, SHOWING STATIC PRESSURE CONTOURS



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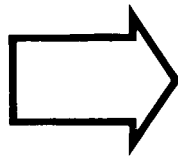
## CHEMICAL REACTING FLOWS

In conclusion, research in the area of Chemical Reacting Flow will lead to an understanding of this complex flow and accurate predictive computer codes. Activity in this topic is focused on three areas: Fluid Mechanics, Combustion Chemistry, and Turbulence-Combustion Interaction. Results from this research will provide important technical "tools we need" to develop new aerospace propulsion systems for the year 2000 and beyond.

## CHEMICAL REACTING FLOWS



FLUID MECHANICS  
COMBUSTION CHEMISTRY  
TURBULENCE—COMBUSTION  
INTERACTION



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